Chemical Examples in Hypergroups

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Abstract Hypergroups first were introduced by Marty in 1934. Up to now many researchers have been working on this field of modern algebra and developed it. It is purpose of this paper to provide examples of hypergroups associated with chemistry. The examples presented are connected to construction from chain reactions.

AMS Subject Classification: 20N20

Keywords and Phrases: hyperstructure, hypergroups, chain relation.

1 Introduction

The theory of algebraic hyperstructures which is a generalization of the concept of algebraic structures first was introduced by Marty in 1934 [4], and had been studied in the following decades and nowadays by many mathematicians, and many papers concerning various hyperstructures have appeared in the literature, for example see [2,3,6,8]. The basic definitions of the object can be found in [1,7].

Definition. A hyperstructure is a non-empty set S together with a function $\cdot : S \times S \longrightarrow P^*(S)$ called hyperoperation, where $P^*(S\}$ denotes the set of all non-empty subsets of S. If $A, B \subseteq S$, $x \in S$ then we define

$$A \cdot B = \bigcup_{a\in A,\, b\in B} a \cdot b, \quad x \cdot B = \{x\} \cdot B, \quad \text{and } A \cdot x = A \cdot \{x\}.$$

The hyperoperation $\cdot$ is called associative in S if

$$(x \cdot y) \cdot z = x \cdot (y \cdot z) \quad \text{for all } x,y,z \text{ in } S.$$

Definition. A hyperstructure $(S , \cdot)$ is called a hypergroup [1] if

i) $(\cdot)$ is associative.

ii) $a \cdot S = S \cdot a = S$ for all $a \in S$.

Definition. A non-empty subset K of the hypergroup S is called a subhypergroup of S if $a \cdot K = K \cdot a = K$ for all $a \in K$.

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In this paper, we will give some examples of hypergroups associated with chemistry. The examples presented are connected to construction from chian reactions.

2 Preliminaries

a) Chain reactions

An atom of group of atoms possessing an odd (unpaired) electron is called a free radical, such as

$$Cl, CH_3, C_2H_5$$

The chlorination of methane is an example of a chain reaction, a reaction that involves a series of steps, each of which generates a reactive substance that brings about the next step. While chain reactions may vary widely in their details, they all have certain fundamental characteristics in common.

1) $Cl_2 \longrightarrow 2Cl^o$

(1) is called Chain-initiating step.

2) $Cl^o + CH_4 \longrightarrow HCl + CH_3{}^o$

3) $CH_3{}^o + Cl_2 \longrightarrow CH_3Cl + Cl^o$

then (2), (3), (2), (3), etc, until finally:

(2) and (3) are called Chain-propagating steps.

4) $Cl^o + Cl^o \longrightarrow Cl_2$ or

5) $CH_3{}^o + CH_3{}^o \longrightarrow CH_3CH_3$ or

6) $CH_3{}^o + Cl^o \longrightarrow CH_3Cl$.

(4),(5) and (6) are called Chain-terminating steps.

First in the chain of reactions is a chain-initiating step, in which energy is absorbed and a reactive particle generated; in the present reaction it is the cleavage of chlorine into atoms (step 1).
There are one or more chain-propagating steps, each of which consumes a reactive particle and generates another; there they are the reaction of chlorine atoms with methane (step 2), and of methyl radicals with chlorine (step 3).

Finally, there are chain-terminating steps, in which reactive particles are consumed but not generated; in the chlorination of methane these would involve the union of two of the reactive particles, or the capture of one of them by the walls of the reaction vessel.

b) The Halogens *F*, *Cl*, *Br*, and *I*

The halogens are all typical non-metals. Although their physical forms differ-fluorine and chlorine are gases, bromine is a liquid and iodine is a solid at room temperature, each consists of diatomic molecules; F_2, Cl_2, Br_2 and I_2. The halogens all react with hydrogen to form gaseous compounds, with the formulas *HF*, *HCl*, *HBr*, and *HI* all of which are very soluble in water. The halogens all react with metals to give halides.

$$:\underset{\cdot\cdot}{\overset{\cdot\cdot}{F}} - \underset{\cdot\cdot}{\overset{\cdot\cdot}{F}}:, \qquad :\underset{\cdot\cdot}{\overset{\cdot\cdot}{Cl}} - \underset{\cdot\cdot}{\overset{\cdot\cdot}{Cl}}:, \qquad :\underset{\cdot\cdot}{\overset{\cdot\cdot}{Br}} - \underset{\cdot\cdot}{\overset{\cdot\cdot}{Br}}:, \qquad :\underset{\cdot\cdot}{\overset{\cdot\cdot}{I}} - \underset{\cdot\cdot}{\overset{\cdot\cdot}{I}}:$$

The reader will find in [5] a deep discussion of chain reactions and halogens.

3 Chemical Hypergroups

In during chain reaction

$$A_2 + B_2 \xleftrightarrow{\text{Heat or Light}} 2AB$$

there exist all molecules A_2, B_2, AB and whose fragment parts A^o, B^o in experiment. Elements of this collection can by combine with each other.

All combinational probability for the set $S = \{A^o, B^o, A_2, B_2, AB\}$ to do without energy can be displayed as follows:

+	A^o	B^o	A_2	B_2	AB
A^o	A^o,A_2	A^o,B^o,AB	A^o,A_2	A^o,B_2,B^o,AB	A^o,AB,A_2,B^o
B^o	A^o, B^o,AB	B^o, B_2	A^o,B^o,AB, A_2	B^o,B_2	A^o, B^o,AB, B_2
A_2	A^o, A_2	A^o, B^o,AB,A_2	A^o, A_2	A^o, B^o,A_2,B_2,AB	A^o, B^o, A_2,AB
B_2	A^o,B^o,B_2,AB	B^o,B_2	A^o, B^o,A_2, B_2,AB	B^o, B_2	A^o, B^o, B_2,AB
AB	A^o,AB,A_2,B^o	A^o,B^o,AB,B_2	A^o, B^o,A_2,AB	A^o, B^o, B_2,AB	A^o, B^o, A_2, B_2,AB

Theorem. (S , +) is a hypergroup.

Proof. Clearly reproduction axiom and associativity are valid. As a sample of how to calculate the associativity, we illustrate some cases:

$$\begin{cases} (AB+A_2)+B_2 = \{ AB, A_2, A^o, B^o \}+B_2 = \{B_2, AB, A_2, A^o, B^o \}, \\ AB+(A_2+B_2)=AB+\{A_2, B_2, A^o, B^o, AB \} = \{ A_2, B_2, AB, A^o, B^o\}, \end{cases}$$

$$\begin{cases} (AB+A^o)+A^o=\{ AB, A^o, A_2, B^o \}+A^o = \{A_2, A^o, AB, B^o \}, \\ AB+(A^o+A^o)=AB+ \{A_2, A^o \} = \{ A_2, AB, A^o, B^o\}, \end{cases}$$

$$\begin{cases} (A_2+B^o)+B_2 = \{ AB, A^o, A_2, B^o \}+B_2 = \{B_2, AB, B^o, A^o, A_2 \}, \\ A_2+(B^o+B_2)=A_2+\{B_2, B^o \} = \{ A_2, A^o, AB, B^o, B_2\}. \end{cases}$$

Corollary. $S_1=\{A^o,A_2\}$ and $S_2=\{B^o,B_2\}$ are only subhypergroups of $(S, +)$.

If we consider A=H and $B \in \{F, Cl, Br, I\}$ (for example B = I), the complete reaction table becomes:

+	H^o	I^o	H_2	I_2	HI
H^o	H^o,H_2	H^o,I^o,HI	H^o,H_2	H^o,I_2,I^o,HI	H^o,HI,H_2,I^o
I^o	H^o, I^o,HI	I^o, I_2	H^o,I^o,HI, H_2	I^o,I_2	H^o, I^o,HI, I_2
H_2	H^o, H_2	H^o, I^o,HI,I_2	H^o, H_2	H^o, I^o,H_2,I_2,HI	H^o, I^o, H_2,HI
I_2	H^o,I^o,I_2,HI	H^o,I_2	H^o, I^o,H_2, I_2,HI	H^o, I_2	H^o, I^o, I_2,HI
HI	H^o,HI,H_2,I^o	H^o,I^o,HI,I_2	H^o, I^o,H_2,HI	H^o, I^o, H_2,HI	H^o, I^o, H_2, I_2,HI

Acknowledgment
We appreciate the assistance and suggestions of Dr. A. Gorgi at the Department of Chemistry.

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